



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:11 AM UTC

PDB ID : 8EOO / pdb_00008eoo
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing human antibodies WRAIR-2063 and WRAIR-2151
Authors : Jensen, J.L.; Sankhala, R.S.; Joyce, M.G.
Deposited on : 2022-10-03
Resolution : 2.77 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

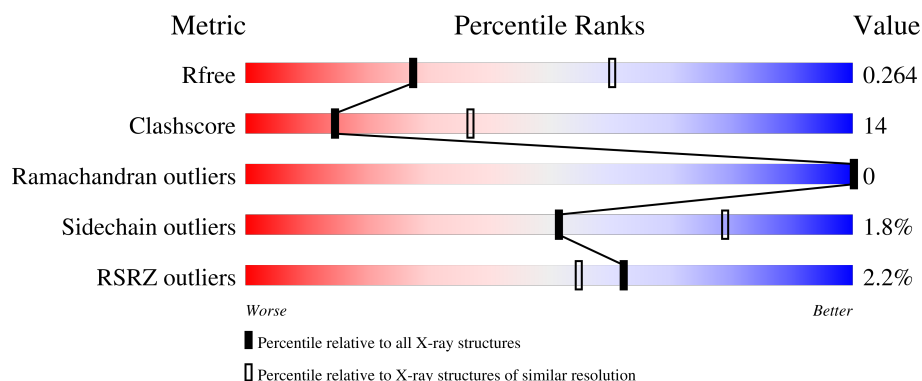
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	% 68% 29% ..
1	F	223	4% 65% 30% ..
2	B	216	76% 22% .
2	K	216	3% 69% 29% ..
3	C	205	2% 73% 21% ..

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Mol	Chain	Length	Quality of chain
3	D	205	 72% 23% .
4	E	227	 3% 76% 22% .
4	H	227	 2% 73% 27%
5	J	219	 3% 72% 26% .
5	L	219	 3% 68% 30% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16527 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called WRAIR-2151 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1639	1046	267	322	4			
1	F	217	Total	C	N	O	S	0	0	0
			1633	1043	266	320	4			

- Molecule 2 is a protein called WRAIR-2151 antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1609	1001	268	335	5			
2	K	214	Total	C	N	O	S	0	0	0
			1618	1006	269	338	5			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	196	Total	C	N	O	S	0	0	0
			1546	990	258	290	8			
3	D	197	Total	C	N	O	S	0	0	0
			1555	997	259	291	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	528	GLY	-	expression tag	UNP P0DTC2
C	529	SER	-	expression tag	UNP P0DTC2
C	530	HIS	-	expression tag	UNP P0DTC2
C	531	HIS	-	expression tag	UNP P0DTC2
C	532	HIS	-	expression tag	UNP P0DTC2
C	533	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	528	GLY	-	expression tag	UNP P0DTC2
D	529	SER	-	expression tag	UNP P0DTC2
D	530	HIS	-	expression tag	UNP P0DTC2
D	531	HIS	-	expression tag	UNP P0DTC2
D	532	HIS	-	expression tag	UNP P0DTC2
D	533	HIS	-	expression tag	UNP P0DTC2
D	534	HIS	-	expression tag	UNP P0DTC2
D	535	HIS	-	expression tag	UNP P0DTC2

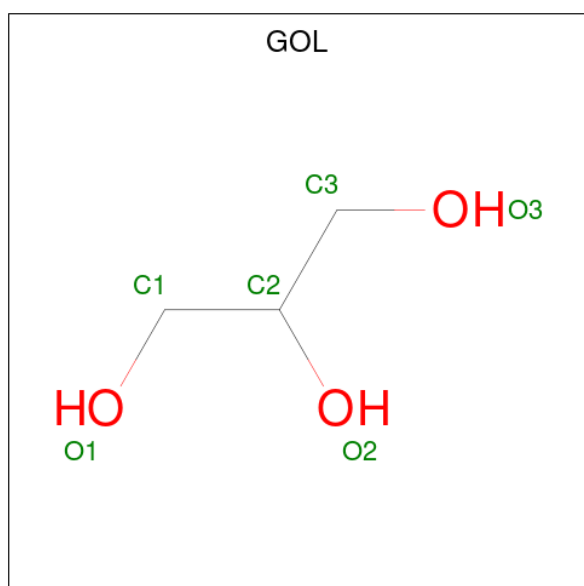
- Molecule 4 is a protein called WRAIR-2063 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	226	Total	C	N	O	S	0	0	0
			1704	1078	287	332	7			
4	H	226	Total	C	N	O	S	0	0	0
			1704	1078	287	332	7			

- Molecule 5 is a protein called WRAIR-2063 antibody Fab light chain.

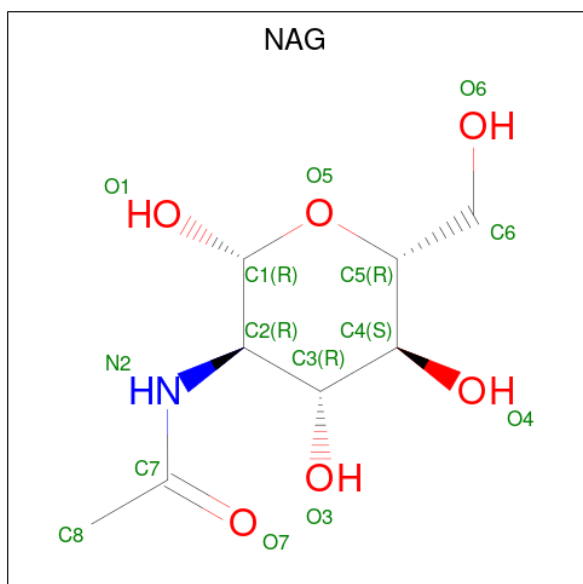
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	219	Total	C	N	O	S	0	0	0
			1692	1055	291	339	7			
5	L	218	Total	C	N	O	S	0	0	0
			1686	1052	290	338	6			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	K	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	7	Total	O	0	0
			7	7		

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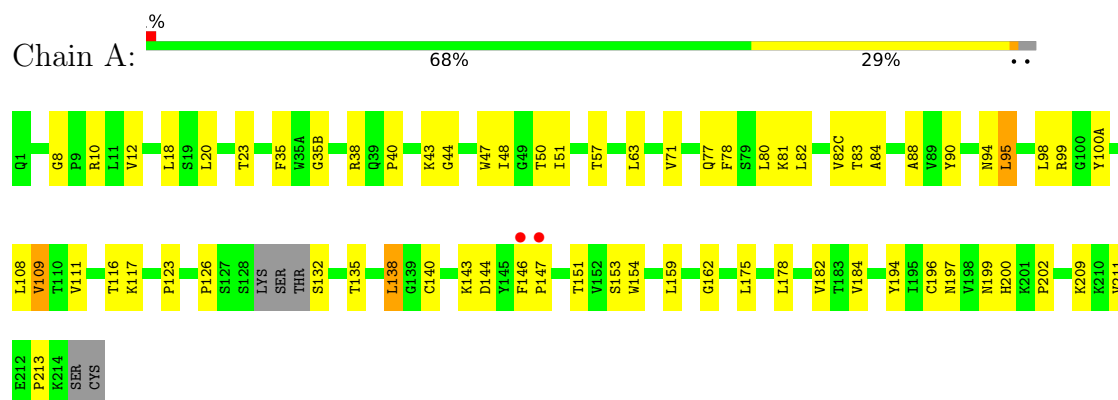
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	8	Total 8	O 8	0	0
8	C	5	Total 5	O 5	0	0
8	D	6	Total 6	O 6	0	0
8	E	10	Total 10	O 10	0	0
8	F	6	Total 6	O 6	0	0
8	H	9	Total 9	O 9	0	0
8	J	11	Total 11	O 11	0	0
8	K	8	Total 8	O 8	0	0
8	L	7	Total 7	O 7	0	0

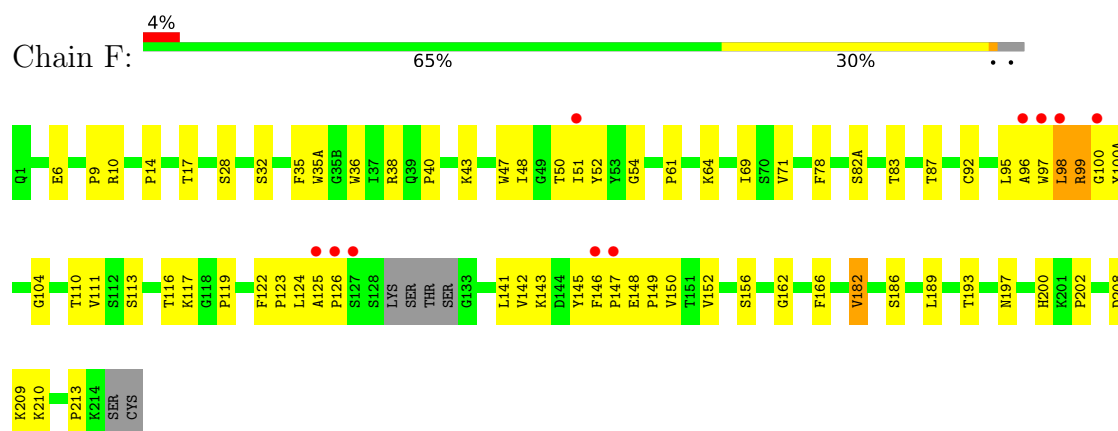
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

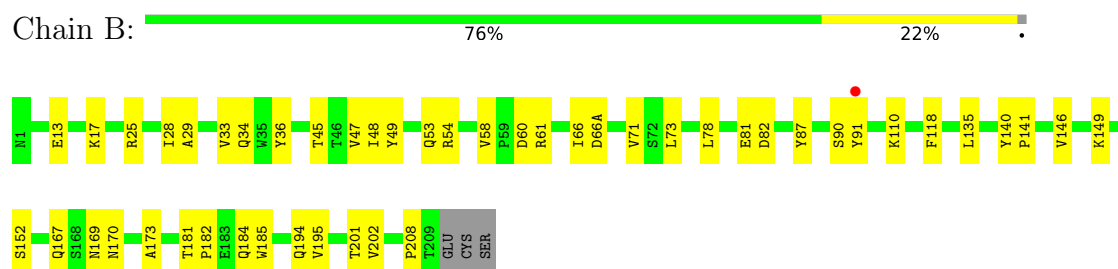
- Molecule 1: WRAIR-2151 antibody Fab heavy chain



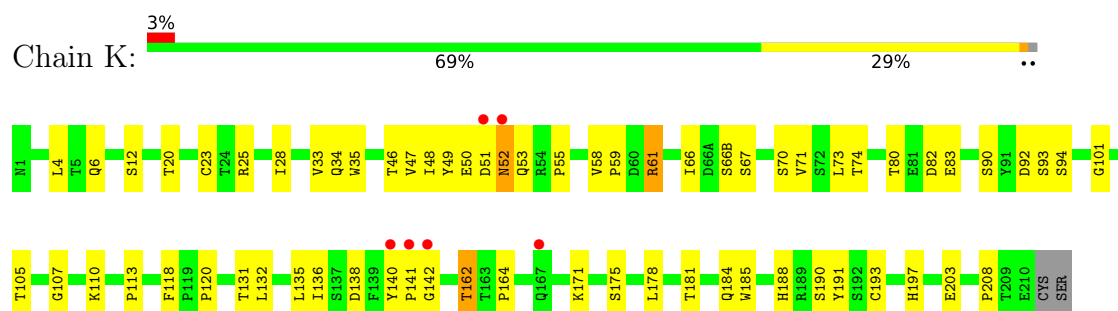
- Molecule 1: WRAIR-2151 antibody Fab heavy chain



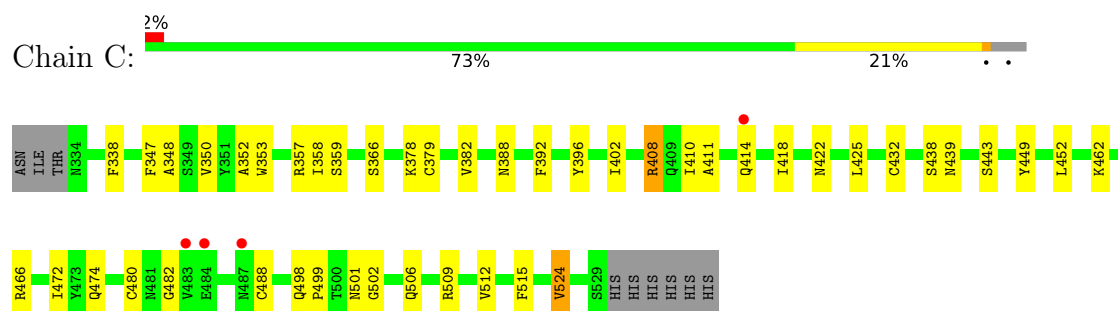
- Molecule 2: WRAIR-2151 antibody Fab light chain



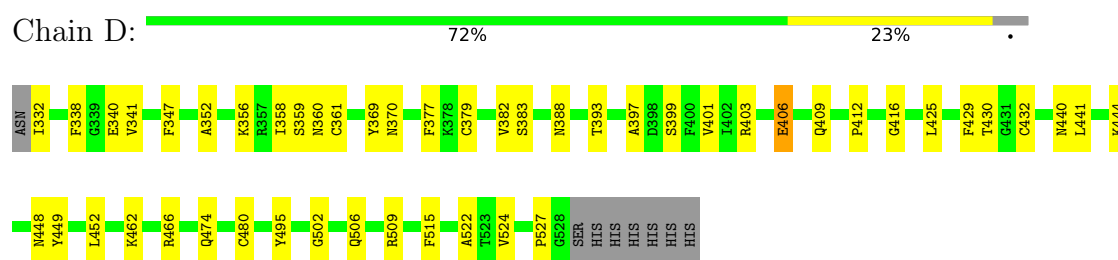
- Molecule 2: WRAIR-2151 antibody Fab light chain



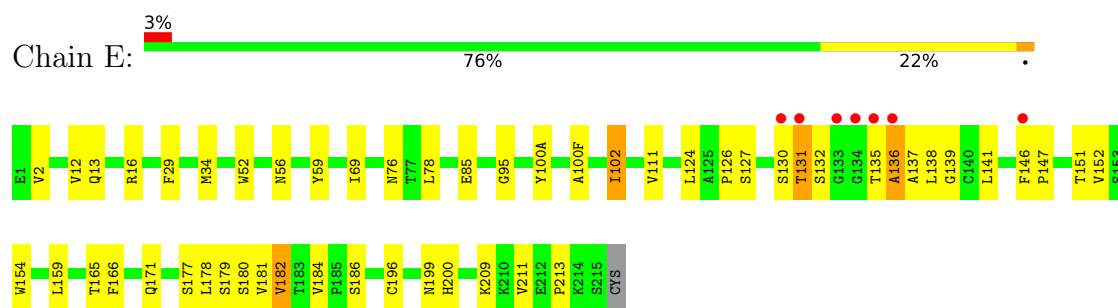
- Molecule 3: Spike protein S1



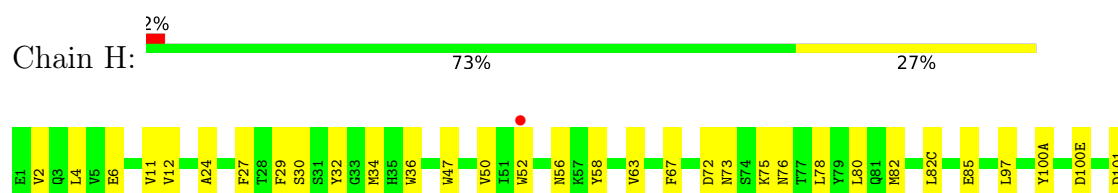
- Molecule 3: Spike protein S1

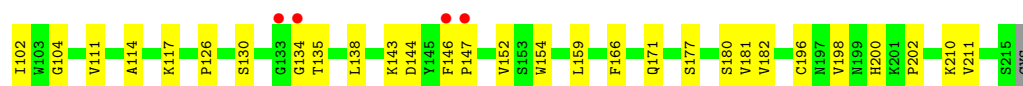


- Molecule 4: WRAIR-2063 antibody Fab heavy chain



- Molecule 4: WRAIR-2063 antibody Fab heavy chain

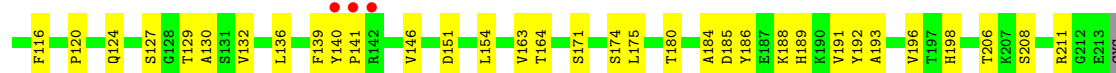




• Molecule 5: WRAIR-2063 antibody Fab light chain



• Molecule 5: WRAIR-2063 antibody Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.07Å 97.41Å 141.13Å 90.00° 99.76° 90.00°	Depositor
Resolution (Å)	19.95 – 2.77 19.95 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.95-2.77) 88.5 (19.95-2.77)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.54 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.194 , 0.255 0.218 , 0.264	Depositor DCC
R_{free} test set	1990 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16527	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/1683	0.59	0/2301
1	F	0.40	0/1677	0.77	3/2293 (0.1%)
2	B	0.45	0/1649	0.71	0/2253
2	K	0.47	1/1658 (0.1%)	0.75	3/2265 (0.1%)
3	C	0.44	0/1590	0.67	1/2164 (0.0%)
3	D	0.41	0/1599	0.66	2/2177 (0.1%)
4	E	0.47	0/1748	0.75	4/2380 (0.2%)
4	H	0.45	0/1748	0.74	0/2380
5	J	0.51	0/1729	0.81	2/2344 (0.1%)
5	L	0.52	0/1723	0.86	3/2336 (0.1%)
All	All	0.45	1/16804 (0.0%)	0.74	18/22893 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	52	ASN	CA-C	6.95	1.61	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	99	ARG	N-CA-C	-7.80	101.20	111.74
1	F	98	LEU	N-CA-C	-7.74	100.95	111.87
1	F	96	ALA	N-CA-C	-6.95	98.71	109.76
3	D	406	GLU	N-CA-C	6.88	121.12	112.87
2	K	52	ASN	CA-C-O	6.77	126.19	119.08
2	K	82	ASP	N-CA-C	6.70	121.31	113.20
3	D	399	SER	N-CA-C	6.31	119.82	109.72
5	L	206	THR	N-CA-C	6.25	118.70	108.52
5	L	61	ARG	N-CA-C	-6.14	104.14	111.69
5	L	95	PRO	N-CA-C	-6.07	105.09	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	95	PRO	N-CA-C	-6.04	105.14	113.53
5	J	206	THR	N-CA-C	5.92	118.06	108.41
4	E	131	THR	CA-C-N	-5.53	113.26	120.44
4	E	131	THR	C-N-CA	-5.53	113.26	120.44
2	K	80	THR	N-CA-C	-5.48	106.44	113.01
4	E	179	SER	N-CA-C	5.34	117.61	108.90
3	C	348	ALA	N-CA-C	5.29	116.91	110.41
4	E	136	ALA	N-CA-C	5.02	117.51	110.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1639	0	1606	53	0
1	F	1633	0	1601	73	0
2	B	1609	0	1540	34	0
2	K	1618	0	1546	51	0
3	C	1546	0	1462	34	0
3	D	1555	0	1473	40	0
4	E	1704	0	1656	39	0
4	H	1704	0	1656	45	0
5	J	1692	0	1644	52	0
5	L	1686	0	1639	53	0
6	B	12	0	16	0	0
6	D	6	0	8	3	0
6	F	6	0	8	0	0
6	K	6	0	8	1	0
6	L	6	0	8	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
8	A	7	0	0	0	0
8	B	8	0	0	0	0
8	C	5	0	0	0	0
8	D	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	10	0	0	0	0
8	F	6	0	0	0	0
8	H	9	0	0	0	0
8	J	11	0	0	0	0
8	K	8	0	0	0	0
8	L	7	0	0	0	0
All	All	16527	0	15897	448	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (448) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:480:CYS:SG	3:C:488:CYS:SG	1.44	1.38
3:D:332:ILE:HD12	3:D:361:CYS:N	1.62	1.12
1:A:51:ILE:HG13	1:A:57:THR:HG22	1.31	1.07
1:F:51:ILE:HG21	1:F:69:ILE:CG2	1.86	1.05
1:F:126:PRO:HG3	1:F:213:PRO:HA	1.39	1.03
1:F:51:ILE:HG21	1:F:69:ILE:HG22	1.44	0.96
1:A:71:VAL:HG12	1:A:78:PHE:HB3	1.47	0.96
1:A:98:LEU:HD23	1:A:99:ARG:HG3	1.49	0.95
1:A:71:VAL:HG12	1:A:78:PHE:CB	1.97	0.94
1:F:98:LEU:HD12	1:F:98:LEU:O	1.70	0.91
5:J:9:LEU:HG	5:J:10:SER:H	1.41	0.85
3:D:332:ILE:HD12	3:D:361:CYS:CA	2.06	0.84
3:D:462:LYS:HB2	5:J:94:TRP:CD1	2.12	0.84
4:E:127:SER:HB2	4:E:130:SER:HB2	1.62	0.81
1:F:51:ILE:CG2	1:F:69:ILE:HG21	2.11	0.81
3:D:332:ILE:CD1	3:D:361:CYS:N	2.42	0.80
1:F:51:ILE:CG2	1:F:69:ILE:CG2	2.61	0.79
1:F:51:ILE:HG21	1:F:69:ILE:HG21	1.66	0.78
1:F:47:TRP:HE1	1:F:50:THR:HG23	1.49	0.77
1:A:51:ILE:HG13	1:A:57:THR:CG2	2.14	0.76
3:D:338:PHE:HE1	3:D:358:ILE:HD13	1.53	0.74
4:H:152:VAL:HG22	4:H:198:VAL:HG22	1.68	0.73
1:A:47:TRP:HE1	1:A:50:THR:HG23	1.52	0.73
4:H:171:GLN:NE2	4:H:177:SER:HB2	2.03	0.72
2:K:47:VAL:O	2:K:48:ILE:HD13	1.90	0.71
4:H:147:PRO:HD2	4:H:200:HIS:CE1	2.26	0.71
4:H:147:PRO:HD2	4:H:200:HIS:HE1	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:410:ILE:O	3:C:425:LEU:HD12	1.91	0.70
5:J:8:PRO:HG2	5:J:21:ILE:HA	1.73	0.70
2:B:48:ILE:HD12	2:B:73:LEU:HD13	1.73	0.70
1:F:156:SER:H	1:F:197:ASN:ND2	1.90	0.70
1:A:100(A):TYR:HB3	2:B:34:GLN:HG2	1.73	0.70
1:A:51:ILE:CG1	1:A:57:THR:HG22	2.17	0.70
5:J:9:LEU:HG	5:J:10:SER:N	2.05	0.70
5:J:9:LEU:O	5:J:102:THR:HG23	1.92	0.69
4:H:34:MET:HB3	4:H:78:LEU:HD22	1.73	0.69
4:E:165:THR:HG22	4:E:178:LEU:HD21	1.73	0.69
3:C:462:LYS:HB2	5:L:94:TRP:CD1	2.28	0.69
2:K:101:GLY:HA3	6:K:301:GOL:H2	1.75	0.69
4:E:136:ALA:HB2	4:E:186:SER:HA	1.74	0.68
5:L:108:ARG:HG3	5:L:171:SER:HB2	1.74	0.68
3:C:480:CYS:CB	3:C:488:CYS:HG	2.00	0.68
2:B:13:GLU:HG3	2:B:17:LYS:HB2	1.76	0.68
4:H:114:ALA:HB3	4:H:146:PHE:CD1	2.28	0.68
1:A:71:VAL:HG12	1:A:78:PHE:HB2	1.76	0.68
5:J:8:PRO:HB2	5:J:102:THR:HG21	1.75	0.68
2:K:34:GLN:HG3	2:K:49:TYR:HA	1.76	0.68
1:F:100(A):TYR:HB3	2:K:34:GLN:HG2	1.76	0.67
3:D:440:ASN:OD1	3:D:441:LEU:HG	1.94	0.67
4:E:138:LEU:HG	4:E:211:VAL:HG11	1.76	0.67
1:A:18:LEU:HD11	1:A:109:VAL:HG21	1.74	0.67
1:F:97:TRP:CH2	1:F:99:ARG:HA	2.29	0.67
2:B:48:ILE:HD12	2:B:73:LEU:CD1	2.25	0.67
1:F:35:PHE:CD1	1:F:97:TRP:HB2	2.29	0.66
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.77	0.66
5:J:141:PRO:HD2	5:J:198:HIS:CE1	2.30	0.65
3:D:332:ILE:HD12	3:D:360:ASN:C	2.22	0.64
5:J:8:PRO:HB2	5:J:102:THR:CG2	2.27	0.64
1:F:98:LEU:HD12	1:F:98:LEU:C	2.22	0.63
5:L:35:TRP:HB2	5:L:48:ILE:HB	1.79	0.63
4:E:2:VAL:HG11	4:E:102:ILE:HD13	1.79	0.63
3:D:370:ASN:OD1	1:F:97:TRP:HB3	1.98	0.63
2:K:52:ASN:C	2:K:52:ASN:OD1	2.42	0.62
2:B:28:ILE:HG12	2:B:71:VAL:HG13	1.82	0.62
4:H:130:SER:HA	5:L:116:PHE:HD1	1.66	0.61
2:B:34:GLN:HG3	2:B:49:TYR:HA	1.81	0.61
4:H:52:TRP:CD1	4:H:56:ASN:HB2	2.35	0.61
1:F:17:THR:HG22	1:F:82(A):SER:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HB3	1:A:48:ILE:HD11	1.83	0.61
4:E:138:LEU:CD2	4:E:154:TRP:CH2	2.85	0.60
2:B:118:PHE:HE2	2:B:135:LEU:HD12	1.65	0.60
1:F:51:ILE:HG23	1:F:69:ILE:HG21	1.83	0.60
5:J:50:LYS:HB2	5:J:53:LYS:HG3	1.83	0.60
2:B:47:VAL:HA	2:B:58:VAL:HG21	1.84	0.60
3:D:338:PHE:CE1	3:D:358:ILE:HD13	2.36	0.60
2:K:140:TYR:HB3	2:K:141:PRO:HD3	1.84	0.60
1:F:38:ARG:HB3	1:F:48:ILE:HD11	1.83	0.60
1:F:35:PHE:HB2	1:F:95:LEU:HB3	1.83	0.60
1:A:138:LEU:CD1	1:A:211:VAL:CG1	2.81	0.59
1:A:138:LEU:HD11	1:A:211:VAL:CG1	2.33	0.59
1:A:138:LEU:HD12	1:A:211:VAL:HG11	1.84	0.59
3:D:370:ASN:HA	1:F:97:TRP:HD1	1.67	0.59
5:L:108:ARG:HB3	5:L:140:TYR:CG	2.38	0.59
5:L:120:PRO:HD3	5:L:132:VAL:HG22	1.84	0.59
3:D:370:ASN:HA	1:F:97:TRP:CD1	2.38	0.58
4:H:32:TYR:CE2	4:H:97:LEU:HB2	2.37	0.58
5:L:7:SER:HB3	5:L:22:SER:H	1.68	0.58
1:A:10:ARG:HH12	1:A:108:LEU:HB3	1.66	0.58
5:L:89:MET:SD	5:L:98:PHE:CE2	2.96	0.58
3:C:338:PHE:HE1	3:C:358:ILE:HD13	1.69	0.58
1:F:126:PRO:HG3	1:F:213:PRO:CA	2.26	0.58
5:L:151:ASP:HA	5:L:191:VAL:CG1	2.34	0.58
1:F:145:TYR:CE2	1:F:150:VAL:CG2	2.87	0.58
5:J:36:PHE:HZ	5:J:89:MET:CE	2.16	0.58
3:D:382:VAL:HG12	3:D:383:SER:O	2.03	0.58
3:D:430:THR:HB	6:D:602:GOL:H12	1.84	0.58
2:K:49:TYR:O	2:K:53:GLN:HB2	2.04	0.58
5:J:187:GLU:HG2	5:J:211:ARG:HH22	1.69	0.57
3:D:474:GLN:HG2	3:D:480:CYS:SG	2.44	0.57
1:F:145:TYR:CE2	1:F:150:VAL:HG21	2.39	0.57
5:J:33:LEU:HB3	5:J:51:VAL:HG22	1.86	0.57
2:K:59:PRO:HB2	2:K:61:ARG:HG3	1.86	0.57
4:H:50:VAL:HG12	4:H:58:TYR:HB2	1.85	0.57
2:K:110:LYS:HA	2:K:140:TYR:HB3	1.87	0.57
1:A:40:PRO:HB2	1:A:43:LYS:HD2	1.86	0.57
1:A:84:ALA:HA	1:A:111:VAL:HG23	1.85	0.57
5:J:36:PHE:CZ	5:J:89:MET:CE	2.87	0.57
1:A:126:PRO:HG3	1:A:138:LEU:HD13	1.87	0.56
1:F:40:PRO:HB2	1:F:43:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:85:GLU:H	4:H:85:GLU:CD	2.14	0.56
2:B:61:ARG:NH1	2:B:82:ASP:OD2	2.32	0.56
4:E:136:ALA:HB3	4:E:184:VAL:HG23	1.88	0.56
5:L:141:PRO:HD2	5:L:198:HIS:CE1	2.40	0.56
4:H:147:PRO:HB2	4:H:202:PRO:HG2	1.88	0.56
5:L:108:ARG:HD3	5:L:140:TYR:HB2	1.88	0.55
2:K:66(B):SER:O	2:K:67:SER:HB2	2.07	0.55
4:E:181:VAL:HG21	5:J:135:LEU:HD22	1.89	0.55
3:D:430:THR:H	6:D:602:GOL:H31	1.72	0.55
4:E:131:THR:HG21	5:J:118:PHE:CE2	2.42	0.55
4:H:52:TRP:CG	4:H:56:ASN:HB2	2.42	0.55
5:J:34:ASN:OD1	5:J:46:ARG:HD2	2.07	0.55
2:B:181:THR:O	2:B:184:GLN:HG2	2.07	0.54
1:A:138:LEU:CD1	1:A:211:VAL:HG11	2.37	0.54
2:K:184:GLN:O	2:K:191:TYR:OH	2.26	0.54
2:K:185:TRP:CZ2	2:K:208:PRO:HA	2.42	0.54
1:F:152:VAL:HA	1:F:197:ASN:O	2.08	0.54
5:J:141:PRO:HD2	5:J:198:HIS:HE1	1.70	0.54
3:D:403:ARG:HD3	3:D:495:TYR:HE1	1.72	0.54
1:F:156:SER:H	1:F:197:ASN:HD21	1.52	0.54
2:K:33:VAL:HG11	2:K:71:VAL:HG21	1.89	0.54
2:B:167:GLN:OE1	2:B:173:ALA:HB2	2.07	0.54
1:F:47:TRP:HE1	1:F:50:THR:CG2	2.20	0.54
4:H:117:LYS:HD3	4:H:144:ASP:O	2.07	0.54
2:K:120:PRO:HB3	2:K:131:THR:H	1.73	0.54
4:H:72:ASP:OD2	4:H:75:LYS:HB2	2.08	0.54
1:F:98:LEU:O	1:F:98:LEU:CD1	2.49	0.53
2:K:49:TYR:HD1	2:K:55:PRO:HD3	1.74	0.53
2:B:149:LYS:HD3	2:B:152:SER:HA	1.91	0.53
2:B:33:VAL:HG11	2:B:71:VAL:HG21	1.89	0.53
5:J:51:VAL:O	5:J:64:GLY:HA3	2.07	0.53
3:C:366:SER:HB3	3:C:388:ASN:HD21	1.72	0.53
4:E:166:PHE:O	4:E:178:LEU:HG	2.09	0.53
5:J:7:SER:HB3	5:J:22:SER:HB3	1.91	0.53
5:J:36:PHE:HZ	5:J:89:MET:HE1	1.71	0.53
5:J:36:PHE:CZ	5:J:89:MET:HE2	2.44	0.53
5:J:35:TRP:CZ3	5:J:88:CYS:HB3	2.43	0.53
2:B:140:TYR:HB3	2:B:141:PRO:HD3	1.91	0.53
2:B:185:TRP:CZ2	2:B:208:PRO:HA	2.44	0.53
4:E:171:GLN:NE2	4:E:177:SER:HB2	2.24	0.52
1:A:35:PHE:HB2	1:A:95:LEU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLY:HA2	2:B:87:TYR:OH	2.09	0.52
2:K:141:PRO:HD2	2:K:197:HIS:NE2	2.24	0.52
3:C:472:ILE:HG13	3:C:482:GLY:O	2.08	0.52
4:E:138:LEU:CD2	4:E:154:TRP:CZ3	2.92	0.52
1:F:166:PHE:CE2	2:K:135:LEU:HD22	2.44	0.52
1:A:126:PRO:HD2	1:A:213:PRO:HA	1.90	0.52
1:A:117:LYS:H	1:A:147:PRO:HD3	1.74	0.52
1:F:162:GLY:O	1:F:182:VAL:HA	2.09	0.52
2:K:47:VAL:HA	2:K:58:VAL:HG21	1.92	0.52
2:K:66:ILE:HG23	2:K:71:VAL:HG12	1.91	0.52
5:L:2:VAL:HG21	5:L:93:HIS:CG	2.44	0.52
4:E:29:PHE:CD2	4:E:76:ASN:HA	2.45	0.52
4:E:131:THR:HG22	5:J:116:PHE:HB3	1.92	0.52
2:B:13:GLU:CG	2:B:17:LYS:HB2	2.39	0.52
5:L:189:HIS:O	5:L:211:ARG:HD3	2.10	0.52
4:E:124:LEU:HD12	4:E:139:GLY:HA3	1.91	0.52
1:F:147:PRO:HB2	1:F:200:HIS:NE2	2.25	0.51
4:H:154:TRP:CZ3	4:H:196:CYS:HB3	2.45	0.51
2:B:33:VAL:HG22	2:B:90:SER:HB2	1.91	0.51
3:C:439:ASN:HD21	3:C:499:PRO:HA	1.73	0.51
3:C:338:PHE:CE1	3:C:358:ILE:HD13	2.45	0.51
4:H:100(E):ASP:OD1	4:H:100(E):ASP:O	2.29	0.51
4:E:52:TRP:CG	4:E:56:ASN:HB2	2.45	0.51
2:K:52:ASN:OD1	2:K:53:GLN:HG2	2.11	0.51
3:D:340:GLU:OE1	3:D:356:LYS:HE2	2.11	0.51
4:E:95:GLY:HA2	4:E:100(F):ALA:HB1	1.92	0.51
5:J:145:LYS:HB3	5:J:197:THR:HB	1.92	0.51
3:C:347:PHE:CD2	3:C:509:ARG:HD3	2.46	0.51
3:C:439:ASN:O	3:C:443:SER:HB2	2.11	0.51
4:H:126:PRO:HG3	4:H:138:LEU:HD12	1.93	0.51
1:A:151:THR:OG1	1:A:199:ASN:HB3	2.10	0.51
1:F:193:THR:CG2	1:F:210:LYS:HE2	2.40	0.51
4:H:159:LEU:HD21	4:H:182:VAL:HG21	1.93	0.51
2:K:35:TRP:CE2	2:K:73:LEU:HB2	2.46	0.51
3:C:462:LYS:HG3	5:L:94:TRP:CG	2.45	0.51
1:F:200:HIS:CD2	1:F:202:PRO:HD2	2.46	0.51
4:H:36:TRP:NE1	4:H:80:LEU:HB2	2.26	0.51
1:F:83:THR:O	1:F:111:VAL:HG21	2.12	0.50
3:C:402:ILE:HD13	3:C:410:ILE:HD11	1.94	0.50
4:E:29:PHE:HE1	4:E:34:MET:HE2	1.77	0.50
4:H:6:GLU:OE2	4:H:104:GLY:HA3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HA	1:A:146:PHE:HD2	1.77	0.50
4:E:159:LEU:HD21	4:E:182:VAL:HG21	1.93	0.50
1:A:80:LEU:HD12	1:A:81:LYS:N	2.26	0.50
3:D:341:VAL:HG11	3:D:397:ALA:HB1	1.94	0.50
1:F:52:TYR:HD2	1:F:54:GLY:H	1.57	0.50
5:J:23:CYS:HB2	5:J:35:TRP:CH2	2.46	0.50
4:H:2:VAL:HG11	4:H:102:ILE:HD13	1.94	0.50
5:J:148:TRP:HB2	5:J:155:GLN:HB2	1.94	0.50
1:A:83:THR:O	1:A:111:VAL:HG21	2.12	0.50
1:F:47:TRP:NE1	1:F:50:THR:HG23	2.23	0.50
1:F:197:ASN:OD1	1:F:208:ASP:OD1	2.30	0.50
4:E:146:PHE:HB3	4:E:147:PRO:HD3	1.94	0.49
4:E:131:THR:HB	4:E:137:ALA:HB3	1.93	0.49
2:K:83:GLU:HG3	2:K:105:THR:HA	1.94	0.49
4:E:147:PRO:HD2	4:E:200:HIS:CE1	2.47	0.49
2:K:25:ARG:HH22	2:K:92:ASP:CG	2.21	0.49
2:K:162:THR:HB	2:K:175:SER:H	1.77	0.49
2:B:167:GLN:HE21	2:B:169:ASN:HB2	1.77	0.49
1:F:117:LYS:H	1:F:147:PRO:HD3	1.77	0.49
3:C:352:ALA:HB1	3:C:466:ARG:HH21	1.78	0.49
1:F:141:LEU:HG	1:F:143:LYS:HG3	1.94	0.49
1:A:200:HIS:CD2	1:A:202:PRO:HD2	2.48	0.49
2:K:188:HIS:O	2:K:208:PRO:HG3	2.13	0.49
2:B:66:ILE:O	2:B:66(A):ASP:OD1	2.30	0.49
2:B:195:VAL:HB	2:B:202:VAL:HG13	1.95	0.48
3:D:352:ALA:C	3:D:466:ARG:HE	2.21	0.48
4:H:4:LEU:HD12	4:H:102:ILE:HG22	1.94	0.48
4:H:12:VAL:O	4:H:111:VAL:HA	2.13	0.48
4:H:134:GLY:O	4:H:135:THR:HG23	2.13	0.48
5:J:9:LEU:CG	5:J:10:SER:H	2.18	0.48
5:L:9:LEU:O	5:L:103:LYS:N	2.46	0.48
1:A:162:GLY:O	1:A:182:VAL:HA	2.13	0.48
2:B:146:VAL:HA	2:B:194:GLN:O	2.13	0.48
5:J:2:VAL:HG21	5:J:93:HIS:CG	2.48	0.48
5:J:94:TRP:HA	5:J:94:TRP:CE3	2.48	0.48
5:J:187:GLU:HA	5:J:211:ARG:HH22	1.78	0.48
4:E:85:GLU:H	4:E:85:GLU:CD	2.21	0.48
4:E:52:TRP:N	4:E:52:TRP:CD1	2.82	0.48
5:J:108:ARG:NH2	5:J:111:ALA:HB2	2.28	0.48
5:J:187:GLU:HA	5:J:211:ARG:NH2	2.29	0.48
1:A:23:THR:HG22	1:A:77:GLN:OE1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:332:ILE:HD13	3:D:360:ASN:HA	1.95	0.48
5:J:124:GLN:HG2	5:J:129:THR:O	2.14	0.48
4:E:34:MET:HB3	4:E:78:LEU:HD22	1.95	0.48
1:A:98:LEU:HD21	2:B:91:TYR:CE2	2.49	0.48
1:F:35:PHE:CE1	1:F:97:TRP:HB2	2.49	0.48
3:C:359:SER:HA	3:C:524:VAL:HG22	1.96	0.47
5:J:48:ILE:HG21	5:J:51:VAL:O	2.14	0.47
1:F:51:ILE:HD13	1:F:69:ILE:CG2	2.43	0.47
2:K:25:ARG:HB2	2:K:28:ILE:HD13	1.96	0.47
1:A:154:TRP:CH2	1:A:196:CYS:HB3	2.49	0.47
3:C:462:LYS:HG3	5:L:94:TRP:CD1	2.49	0.47
1:F:87:THR:HG23	1:F:110:THR:HA	1.96	0.47
4:H:50:VAL:CG1	4:H:58:TYR:HB2	2.44	0.47
3:D:382:VAL:HG12	3:D:383:SER:N	2.30	0.47
1:F:100:GLY:O	2:K:34:GLN:NE2	2.48	0.47
5:J:89:MET:SD	5:J:98:PHE:CE2	3.08	0.47
3:D:403:ARG:HD3	3:D:495:TYR:CE1	2.50	0.47
4:E:151:THR:OG1	4:E:199:ASN:HB3	2.15	0.47
1:F:61:PRO:HA	1:F:64:LYS:HG3	1.96	0.47
5:L:151:ASP:OD1	5:L:191:VAL:HG12	2.15	0.47
1:A:8:GLY:HA3	1:A:20:LEU:HD23	1.97	0.47
1:A:80:LEU:HD12	1:A:81:LYS:H	1.79	0.46
2:K:49:TYR:O	2:K:50:GLU:HB2	2.16	0.46
5:L:193:ALA:HB2	5:L:208:SER:HB3	1.96	0.46
4:E:132:SER:O	4:E:135:THR:O	2.33	0.46
1:F:28:SER:O	1:F:32:SER:HB3	2.14	0.46
1:F:145:TYR:CE2	1:F:150:VAL:HG23	2.51	0.46
1:F:193:THR:HG23	1:F:210:LYS:HE2	1.96	0.46
5:L:184:ALA:O	5:L:188:LYS:HG3	2.15	0.46
3:D:412:PRO:HG3	3:D:429:PHE:HB3	1.97	0.46
1:F:116:THR:HG23	1:F:147:PRO:HG2	1.97	0.46
5:J:147:GLN:O	5:J:194:CYS:HA	2.16	0.46
2:K:73:LEU:HD12	2:K:74:THR:N	2.30	0.46
5:L:108:ARG:HB3	5:L:140:TYR:CD1	2.51	0.46
5:L:136:LEU:HB3	5:L:139:PHE:CE1	2.50	0.46
3:C:350:VAL:O	3:C:353:TRP:HD1	1.99	0.46
5:J:8:PRO:CG	5:J:21:ILE:HA	2.45	0.46
5:L:163:VAL:HG22	5:L:164:THR:N	2.31	0.46
5:J:108:ARG:HD2	5:J:170:ASP:O	2.15	0.46
1:F:97:TRP:CE3	1:F:97:TRP:HA	2.50	0.46
1:A:12:VAL:O	1:A:111:VAL:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:401:VAL:HG22	3:D:509:ARG:HG2	1.98	0.46
3:D:388:ASN:HD22	3:D:527:PRO:HD2	1.81	0.45
1:F:156:SER:N	1:F:197:ASN:HD21	2.13	0.45
3:C:408:ARG:HH11	3:C:408:ARG:HB2	1.80	0.45
1:A:143:LYS:HB3	1:A:143:LYS:HE3	1.76	0.45
2:B:29:ALA:O	3:C:378:LYS:HE3	2.15	0.45
4:H:130:SER:HA	5:L:116:PHE:CD1	2.49	0.45
2:K:35:TRP:CD2	2:K:73:LEU:HB2	2.50	0.45
5:L:94:TRP:CE3	5:L:94:TRP:HA	2.50	0.45
5:L:136:LEU:HD21	5:L:196:VAL:HG13	1.98	0.45
1:A:132:SER:HB2	1:A:135:THR:OG1	2.17	0.45
3:D:393:THR:HA	3:D:522:ALA:HA	1.97	0.45
4:E:138:LEU:HD23	4:E:154:TRP:CH2	2.51	0.45
3:D:379:CYS:HA	3:D:432:CYS:HA	1.99	0.45
1:F:9:PRO:O	1:F:10:ARG:HB2	2.17	0.45
1:F:147:PRO:HD2	1:F:200:HIS:CE1	2.50	0.45
2:K:132:LEU:HD13	2:K:178:LEU:HD23	1.98	0.45
1:A:144:ASP:HB3	1:A:175:LEU:HD13	1.99	0.45
3:C:350:VAL:HG22	3:C:422:ASN:HB3	1.99	0.45
5:J:27(D):TYR:CG	5:J:27(E):SER:N	2.84	0.45
5:L:108:ARG:CD	5:L:140:TYR:HB2	2.47	0.45
5:J:146:VAL:HG12	5:J:196:VAL:HG22	1.98	0.45
3:C:379:CYS:HB3	3:C:382:VAL:HG23	1.98	0.45
4:E:209:LYS:HA	4:E:209:LYS:HD3	1.79	0.45
2:K:47:VAL:O	2:K:55:PRO:HD2	2.17	0.45
2:K:193:CYS:O	2:K:203:GLU:HA	2.16	0.45
3:C:418:ILE:HA	3:C:422:ASN:HD22	1.82	0.45
3:C:502:GLY:O	3:C:506:GLN:HG3	2.17	0.45
2:B:140:TYR:CD1	2:B:140:TYR:C	2.92	0.44
3:C:357:ARG:HG3	3:C:396:TYR:CE2	2.52	0.44
3:C:474:GLN:HG2	3:C:480:CYS:SG	2.57	0.44
1:F:14:PRO:HD2	1:F:113:SER:OG	2.17	0.44
1:F:97:TRP:CZ3	1:F:99:ARG:HA	2.52	0.44
1:F:123:PRO:HG3	1:F:209:LYS:NZ	2.32	0.44
5:J:36:PHE:CE2	5:J:89:MET:HE2	2.52	0.44
5:J:192:TYR:HB2	5:J:209:PHE:CZ	2.53	0.44
5:L:186:TYR:O	5:L:192:TYR:OH	2.36	0.44
1:A:123:PRO:HD3	1:A:209:LYS:HZ3	1.82	0.44
3:D:425:LEU:HD23	3:D:425:LEU:HA	1.85	0.44
4:H:52:TRP:CH2	4:H:100(A):TYR:CD1	3.05	0.44
3:D:444:LYS:HG2	3:D:448:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:515:PHE:O	6:D:602:GOL:H11	2.18	0.44
1:F:36:TRP:CZ3	1:F:92:CYS:HB3	2.53	0.44
5:J:142:ARG:HB2	5:J:173:TYR:CE2	2.53	0.44
5:L:124:GLN:O	5:L:127:SER:HB3	2.18	0.44
1:A:35(B):GLY:HA2	1:A:50:THR:HA	2.00	0.44
4:H:143:LYS:HG2	4:H:144:ASP:N	2.32	0.44
2:K:46:THR:HG22	2:K:55:PRO:HG3	1.99	0.44
5:L:54:ARG:NE	5:L:60:ASP:HA	2.32	0.44
2:K:20:THR:HG22	2:K:74:THR:OG1	2.18	0.44
3:C:411:ALA:O	3:C:414:GLN:HB2	2.17	0.43
1:F:100(A):TYR:CB	2:K:34:GLN:HG2	2.46	0.43
1:A:138:LEU:CD1	1:A:211:VAL:HG12	2.48	0.43
3:C:472:ILE:HG22	3:C:488:CYS:HB3	1.99	0.43
3:D:409:GLN:NE2	3:D:416:GLY:HA3	2.33	0.43
1:F:35:PHE:CE1	1:F:52:TYR:CD1	3.06	0.43
5:L:3:VAL:HB	5:L:26:SER:HB3	2.00	0.43
5:L:27(D):TYR:CG	5:L:27(E):SER:N	2.86	0.43
1:A:18:LEU:HB3	1:A:82:LEU:HB3	2.00	0.43
1:A:94:ASN:C	1:A:94:ASN:OD1	2.61	0.43
2:B:54:ARG:NE	2:B:60:ASP:HA	2.34	0.43
1:F:35(A):TRP:HB3	1:F:78:PHE:CZ	2.53	0.43
4:H:180:SER:C	4:H:181:VAL:HG13	2.42	0.43
5:J:37:GLN:HB2	5:J:47:LEU:HD11	2.00	0.43
2:K:23:CYS:O	2:K:70:SER:HA	2.19	0.43
5:L:48:ILE:HD13	5:L:54:ARG:HA	2.00	0.43
4:H:143:LYS:HG3	4:H:177:SER:OG	2.18	0.43
5:J:8:PRO:HG2	5:J:21:ILE:HG23	1.99	0.43
4:E:13:GLN:HB2	4:E:16:ARG:HD3	2.00	0.43
4:H:29:PHE:CD2	4:H:76:ASN:HA	2.54	0.43
5:L:108:ARG:CB	5:L:140:TYR:CD1	3.02	0.43
4:E:52:TRP:CD1	4:E:56:ASN:HB2	2.54	0.43
4:E:124:LEU:HD21	4:E:141:LEU:HB2	2.00	0.43
3:D:359:SER:HA	3:D:524:VAL:CG2	2.49	0.43
1:F:147:PRO:HB2	1:F:202:PRO:HG2	1.99	0.43
4:H:47:TRP:HB2	5:L:98:PHE:HE1	1.84	0.43
2:K:113:PRO:HD3	2:K:197:HIS:ND1	2.34	0.43
5:L:33:LEU:HA	5:L:89:MET:O	2.19	0.43
5:L:185:ASP:HA	5:L:188:LYS:HD2	2.01	0.43
3:C:379:CYS:HA	3:C:432:CYS:HA	1.99	0.43
4:E:52:TRP:HZ3	4:E:100(A):TYR:CD2	2.37	0.43
4:E:165:THR:CG2	4:E:178:LEU:HD21	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:425:LEU:HD21	3:C:512:VAL:HG11	2.01	0.42
1:F:124:LEU:HD21	1:F:141:LEU:HB2	2.01	0.42
1:F:125:ALA:HB3	2:K:118:PHE:HD1	1.84	0.42
4:H:24:ALA:HB1	4:H:27:PHE:CE1	2.54	0.42
1:A:88:ALA:HB3	1:A:90:TYR:CE1	2.54	0.42
1:F:189:LEU:HD23	1:F:189:LEU:HA	1.87	0.42
5:J:125:LEU:HD23	5:J:125:LEU:HA	1.86	0.42
2:K:4:LEU:HB3	2:K:23:CYS:SG	2.59	0.42
2:K:181:THR:OG1	2:K:184:GLN:HG2	2.20	0.42
3:D:502:GLY:O	3:D:506:GLN:HG3	2.20	0.42
2:K:190:SER:HA	2:K:208:PRO:HD3	2.01	0.42
5:L:108:ARG:NE	5:L:140:TYR:HB2	2.34	0.42
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.79	0.42
3:D:403:ARG:HG2	3:D:406:GLU:CD	2.44	0.42
1:F:51:ILE:HD13	1:F:69:ILE:HG22	2.01	0.42
4:H:101:ASP:O	4:H:102:ILE:HG13	2.19	0.42
1:A:82(C):VAL:HG22	1:A:111:VAL:HG11	2.02	0.42
2:B:110:LYS:HA	2:B:140:TYR:HB3	2.01	0.42
5:J:6:GLN:HA	5:J:22:SER:O	2.19	0.42
5:L:139:PHE:HZ	5:L:175:LEU:HB2	1.83	0.42
3:D:347:PHE:CE2	3:D:509:ARG:HB3	2.55	0.42
2:K:73:LEU:HD12	2:K:74:THR:H	1.85	0.42
1:A:153:SER:OG	1:A:197:ASN:HB2	2.20	0.42
1:A:159:LEU:HD21	1:A:182:VAL:HG21	2.01	0.42
2:B:36:TYR:HA	2:B:45:THR:O	2.20	0.42
1:F:35:PHE:CE1	1:F:52:TYR:HD1	2.38	0.42
4:H:82:MET:HB3	4:H:82(C):LEU:HD21	2.02	0.42
5:L:47:LEU:HA	5:L:58:VAL:HG21	2.02	0.42
1:F:119:PRO:HB2	1:F:142:VAL:HG13	2.01	0.42
4:H:63:VAL:HB	4:H:67:PHE:CG	2.55	0.42
5:J:125:LEU:O	5:J:183:LYS:HD2	2.19	0.42
2:K:93:SER:OG	2:K:94:SER:N	2.53	0.42
5:L:6:GLN:HE21	5:L:6:GLN:HB3	1.66	0.42
1:F:146:PHE:HB3	1:F:147:PRO:HD3	2.01	0.41
5:J:6:GLN:HE21	5:J:6:GLN:HB3	1.68	0.41
5:L:37:GLN:CB	5:L:47:LEU:HD11	2.46	0.41
1:A:184:VAL:HG11	1:A:194:TYR:CE1	2.55	0.41
4:E:152:VAL:HG11	4:E:180:SER:CB	2.50	0.41
2:K:138:ASP:HA	2:K:171:LYS:HD3	2.00	0.41
5:L:50:LYS:O	5:L:52:SER:N	2.46	0.41
5:L:124:GLN:HG2	5:L:129:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:GLU:H	2:B:81:GLU:HG2	1.72	0.41
5:J:9:LEU:O	5:J:102:THR:CG2	2.65	0.41
5:L:130:ALA:O	5:L:180:THR:HA	2.20	0.41
1:A:10:ARG:NH2	1:A:108:LEU:H	2.19	0.41
3:C:498:GLN:HB2	3:C:501:ASN:ND2	2.35	0.41
1:F:122:PHE:CD2	1:F:143:LYS:HD3	2.56	0.41
2:K:25:ARG:HB2	2:K:28:ILE:CD1	2.50	0.41
3:C:449:TYR:CD2	3:D:452:LEU:HD11	2.55	0.41
4:E:126:PRO:HG2	4:E:213:PRO:HB3	2.03	0.41
4:H:134:GLY:O	4:H:135:THR:CG2	2.69	0.41
5:L:13:VAL:HG21	5:L:78:VAL:HG11	2.01	0.41
3:C:392:PHE:CD1	3:C:515:PHE:HB3	2.55	0.41
3:C:462:LYS:HB2	5:L:94:TRP:NE1	2.35	0.41
4:H:30:SER:HA	4:H:73:ASN:ND2	2.36	0.41
4:H:138:LEU:HG	4:H:211:VAL:HG11	2.02	0.41
4:H:166:PHE:HE2	5:L:174:SER:O	2.04	0.41
5:L:35:TRP:CE2	5:L:73:LEU:HB2	2.56	0.41
5:L:111:ALA:O	5:L:139:PHE:HA	2.20	0.41
1:A:35:PHE:CZ	1:A:98:LEU:HB2	2.55	0.41
3:D:382:VAL:HG12	3:D:383:SER:C	2.46	0.41
4:E:154:TRP:CH2	4:E:196:CYS:HB3	2.55	0.41
1:F:6:GLU:OE2	1:F:104:GLY:HA3	2.21	0.41
4:H:27:PHE:CE2	4:H:29:PHE:HA	2.55	0.41
5:J:94:TRP:N	5:J:95:PRO:CD	2.84	0.41
2:K:28:ILE:HG12	2:K:71:VAL:HG13	2.03	0.41
3:D:369:TYR:HB3	3:D:377:PHE:CZ	2.56	0.41
4:E:12:VAL:O	4:E:111:VAL:HA	2.20	0.41
5:J:95:PRO:HB2	5:J:97:THR:HG23	2.03	0.41
1:A:95:LEU:HD12	1:A:100(A):TYR:C	2.46	0.40
2:B:54:ARG:HE	2:B:60:ASP:HA	1.86	0.40
2:B:181:THR:HG23	2:B:182:PRO:HD2	2.03	0.40
1:F:156:SER:N	1:F:197:ASN:ND2	2.64	0.40
4:H:2:VAL:HG13	4:H:27:PHE:CD1	2.56	0.40
2:K:185:TRP:CH2	2:K:208:PRO:HA	2.56	0.40
1:A:140:CYS:SG	1:A:154:TRP:CH2	3.15	0.40
4:E:59:TYR:CZ	4:E:69:ILE:HG22	2.57	0.40
2:K:107:GLY:N	2:K:140:TYR:OH	2.49	0.40
3:C:452:LEU:HD11	3:D:449:TYR:CD1	2.56	0.40
1:F:98:LEU:HD11	1:F:100:GLY:CA	2.51	0.40
1:F:148:GLU:N	1:F:149:PRO:HD2	2.36	0.40
4:H:11:VAL:HG11	4:H:146:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:142:GLY:O	2:K:164:PRO:HG2	2.21	0.40
2:B:48:ILE:HA	2:B:53:GLN:O	2.22	0.40
3:D:382:VAL:CG1	3:D:383:SER:N	2.85	0.40
1:F:145:TYR:CD2	1:F:150:VAL:HG21	2.56	0.40
4:H:154:TRP:CH2	4:H:196:CYS:HB3	2.55	0.40
5:L:140:TYR:HB3	5:L:141:PRO:HD3	2.02	0.40
1:A:147:PRO:HB2	1:A:200:HIS:NE2	2.36	0.40
2:B:184:GLN:HE21	2:B:184:GLN:HB3	1.52	0.40
2:K:12:SER:HA	2:K:105:THR:O	2.22	0.40
5:L:9:LEU:HA	5:L:102:THR:HA	2.03	0.40
5:L:90:GLN:NE2	5:L:96:LEU:HA	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/223 (96%)	200 (94%)	14 (6%)	0	100	100
1	F	213/223 (96%)	202 (95%)	11 (5%)	0	100	100
2	B	211/216 (98%)	204 (97%)	7 (3%)	0	100	100
2	K	212/216 (98%)	202 (95%)	10 (5%)	0	100	100
3	C	194/205 (95%)	185 (95%)	9 (5%)	0	100	100
3	D	195/205 (95%)	186 (95%)	9 (5%)	0	100	100
4	E	224/227 (99%)	214 (96%)	10 (4%)	0	100	100
4	H	224/227 (99%)	219 (98%)	5 (2%)	0	100	100
5	J	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
5	L	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
All	All	2120/2180 (97%)	2034 (96%)	86 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/191 (97%)	181 (97%)	5 (3%)	39	71
1	F	185/191 (97%)	182 (98%)	3 (2%)	55	81
2	B	186/189 (98%)	183 (98%)	3 (2%)	55	81
2	K	187/189 (99%)	181 (97%)	6 (3%)	34	67
3	C	168/177 (95%)	165 (98%)	3 (2%)	51	79
3	D	169/177 (96%)	169 (100%)	0	100	100
4	E	189/190 (100%)	187 (99%)	2 (1%)	65	85
4	H	189/190 (100%)	188 (100%)	1 (0%)	81	92
5	J	194/194 (100%)	189 (97%)	5 (3%)	40	72
5	L	193/194 (100%)	187 (97%)	6 (3%)	35	68
All	All	1846/1882 (98%)	1812 (98%)	34 (2%)	51	79

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	95	LEU
1	A	109	VAL
1	A	138	LEU
1	A	178	LEU
2	B	25	ARG
2	B	170	ASN
2	B	201	THR
3	C	408	ARG
3	C	438	SER
3	C	524	VAL
4	E	102	ILE
4	E	182	VAL
1	F	71	VAL

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Mol	Chain	Res	Type
1	F	182	VAL
1	F	186	SER
4	H	210	LYS
5	J	55	ASP
5	J	108	ARG
5	J	162	SER
5	J	191	VAL
5	J	211	ARG
2	K	6	GLN
2	K	51	ASP
2	K	61	ARG
2	K	90	SER
2	K	136	ILE
2	K	162	THR
5	L	6	GLN
5	L	7	SER
5	L	11	LEU
5	L	33	LEU
5	L	146	VAL
5	L	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
2	B	34	GLN
2	B	38	GLN
2	B	126	GLN
2	B	167	GLN
3	C	370	ASN
3	C	498	GLN
4	E	56	ASN
4	E	164	HIS
1	F	171	GLN
1	F	197	ASN
5	J	147	GLN
2	K	108	GLN
2	K	170	ASN
5	L	17	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	C	601	3	14,14,15	1.35	2 (14%)	17,19,21	0.97	1 (5%)
6	GOL	B	302	-	5,5,5	1.11	0	5,5,5	0.90	0
7	NAG	D	601	3	14,14,15	0.29	0	17,19,21	0.59	0
6	GOL	F	301	-	5,5,5	0.93	0	5,5,5	1.07	0
6	GOL	B	301	-	5,5,5	0.09	0	5,5,5	0.31	0
6	GOL	K	301	-	5,5,5	0.09	0	5,5,5	0.35	0
6	GOL	D	602	-	5,5,5	0.08	0	5,5,5	0.31	0
6	GOL	L	301	-	5,5,5	0.92	0	5,5,5	1.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	601	3	-	4/6/23/26	0/1/1/1
6	GOL	B	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	601	3	-	2/6/23/26	0/1/1/1
6	GOL	F	301	-	-	2/4/4/4	-
6	GOL	B	301	-	-	2/4/4/4	-
6	GOL	K	301	-	-	2/4/4/4	-
6	GOL	D	602	-	-	2/4/4/4	-
6	GOL	L	301	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	601	NAG	C1-C2	3.60	1.57	1.52
7	C	601	NAG	O5-C1	3.30	1.49	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	601	NAG	C1-O5-C5	3.29	116.60	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	302	GOL	O1-C1-C2-O2
6	B	302	GOL	O1-C1-C2-C3
6	D	602	GOL	C1-C2-C3-O3
6	K	301	GOL	C1-C2-C3-O3
7	C	601	NAG	O5-C5-C6-O6
7	C	601	NAG	C4-C5-C6-O6
7	C	601	NAG	C8-C7-N2-C2
7	C	601	NAG	O7-C7-N2-C2
7	D	601	NAG	C8-C7-N2-C2
7	D	601	NAG	O7-C7-N2-C2
6	F	301	GOL	O2-C2-C3-O3
6	K	301	GOL	O2-C2-C3-O3
6	F	301	GOL	C1-C2-C3-O3
6	L	301	GOL	O1-C1-C2-C3
6	D	602	GOL	O2-C2-C3-O3
6	L	301	GOL	O1-C1-C2-O2
6	B	301	GOL	C1-C2-C3-O3
6	B	301	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	301	GOL	1	0
6	D	602	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/223 (97%)	-0.07	2 (0%) 81 76	66, 93, 128, 169	0
1	F	217/223 (97%)	0.08	10 (4%) 37 31	77, 99, 131, 210	0
2	B	213/216 (98%)	-0.15	1 (0%) 87 83	61, 84, 126, 155	0
2	K	214/216 (99%)	0.01	6 (2%) 55 47	72, 96, 140, 178	0
3	C	196/205 (95%)	-0.03	4 (2%) 65 58	66, 87, 149, 180	0
3	D	197/205 (96%)	-0.11	0 100 100	69, 87, 144, 176	0
4	E	226/227 (99%)	-0.15	7 (3%) 51 44	64, 85, 116, 210	0
4	H	226/227 (99%)	-0.21	5 (2%) 62 55	63, 82, 114, 153	0
5	J	219/219 (100%)	-0.09	6 (2%) 56 48	63, 83, 118, 173	0
5	L	218/219 (99%)	-0.00	7 (3%) 50 43	70, 83, 104, 131	0
All	All	2144/2180 (98%)	-0.07	48 (2%) 62 55	61, 88, 129, 210	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	94	TRP	6.2
5	L	140	TYR	5.8
5	L	94	TRP	5.5
1	A	147	PRO	4.6
2	K	51	ASP	4.3
4	H	147	PRO	4.2
5	L	7	SER	3.9
1	F	146	PHE	3.6
1	F	98	LEU	3.5
1	A	146	PHE	3.5
4	H	146	PHE	3.5
5	J	96	LEU	3.3
5	L	141	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
4	E	134	GLY	3.1
1	F	100	GLY	3.1
5	L	9	LEU	3.1
4	E	136	ALA	2.9
5	J	93	HIS	2.9
4	E	131	THR	2.8
3	C	483	VAL	2.8
4	E	130	SER	2.6
5	J	95	PRO	2.6
4	E	146	PHE	2.6
1	F	127	SER	2.5
1	F	125	ALA	2.5
2	K	52	ASN	2.5
4	E	135	THR	2.5
2	K	142	GLY	2.4
2	K	140	TYR	2.4
5	J	89	MET	2.4
4	H	134	GLY	2.4
1	F	96	ALA	2.4
1	F	126	PRO	2.3
1	F	147	PRO	2.3
1	F	51	ILE	2.2
3	C	414	GLN	2.2
1	F	97	TRP	2.2
3	C	484	GLU	2.2
4	H	52	TRP	2.1
2	B	91	TYR	2.1
2	K	167	GLN	2.1
4	E	133	GLY	2.1
2	K	141	PRO	2.1
5	J	9	LEU	2.1
4	H	133	GLY	2.1
3	C	487	ASN	2.1
5	L	27(E)	SER	2.0
5	L	142	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	D	601	14/15	0.46	0.14	116,130,134,134	0
6	GOL	K	301	6/6	0.62	0.18	86,89,91,93	0
6	GOL	D	602	6/6	0.65	0.18	84,88,91,95	0
6	GOL	B	302	6/6	0.70	0.11	99,104,106,108	0
7	NAG	C	601	14/15	0.73	0.11	101,113,116,118	0
6	GOL	B	301	6/6	0.79	0.17	80,85,86,90	0
6	GOL	L	301	6/6	0.81	0.14	79,83,85,86	0
6	GOL	F	301	6/6	0.82	0.10	81,84,86,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.